Introduction To Quantum Mechanics

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Contents

Acknowledgement

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1 The Wave Function

What we are looking for is the **wave function $\boldsymbol{\Psi}$**.

Law 1.1 (Schrodinger Equation).

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi.$$

For simplicity, we always rewrite it as:

$$i\hbar\partial_t\Psi = -\frac{\hbar^2}{2m}\partial_x^2\Psi + V\Psi.$$

Born's statistical interpretation:

$$\int_a^b |\Psi(x,t)|^2 \,\mathrm{d}x = \text{probability of finding the particle between } a \text{ and } b \text{ at time } t.$$

Law 1.2 (Normalization).

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \,\mathrm{d}x = 1.$$

Proposition 1.1. The wave function will always stay NORMALIZED.

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \,\mathrm{d}x = 0.$$

Proof. By Schrodinger EQ.,

$$\text{LHS} = \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\Bigg|_{-\infty}^{+\infty}.$$

□

Definition 1.1.

$$\langle x\rangle \xlongequal{def} \int_{-\infty}^{\infty} x|\Psi|^2 \,\mathrm{d}x$$

and

$$\langle p\rangle \xlongequal{def} m\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t}.$$

Theorem 1.1.

$$\langle x\rangle = \int \Psi^*(x)\Psi \,\mathrm{d}x$$

and

$$\langle p\rangle = \int \Psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi \,\mathrm{d}x.$$

Remark 1.1 (Operator)**.** We say that the operator x represents position, and the operator $-i\hbar\,\partial/\partial x$ represents momentum. Also,

$$\langle Q(x,p)\rangle = \int_{-\infty}^{\infty} \Psi^* \left[Q(x, -i\hbar\frac{\partial}{\partial x}) \right] \Psi \,\mathrm{d}x.$$

Property 1.1. Operators do **NOT**, in general, commute. For example, $\hat{x}\hat{p} \neq \hat{p}\hat{x}$, i.e.,

$$\exists \text{ a function } f, \text{ s.t. } (\hat{x}\hat{p})f \neq (\hat{p}\hat{x})f.$$

Theorem 1.2 (de Broglie formula)**.** The wave length is related to the momentum of the particle:

$$p = \frac{h}{\lambda} = \frac{2\pi\hbar}{\lambda}.$$

Theorem 1.3 (Heisenberg's uncertainty principle)**.**

$$\sigma_x\sigma_p \geq \frac{\hbar}{2}.$$

2 Time-independent Schrodinger Equation

2.1 Stationary states

We look for solutions that are simple products,

$$\Psi(x,t) = \psi(x)\varphi(t).$$

Theorem 2.1. By the method of separation of variables,

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V\psi = E\psi$$

and

$$\varphi(t) = e^{-iEt/\hbar}.$$

The first is called the **time-independent Schrodinger equation**.

Definition 2.1 (Hamiltonian)**.** In classical mechanics, the total energy (kinetic plus potential) is called Hamiltonian:

$$H(x,p) = \frac{p^2}{2m} + V(x).$$

Now we introduce **Hamiltonian operator**:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x).$$

Thus the time-independent Schrodinger EQ. can be written

$$\hat{H}\psi = E\psi$$

which is **IMPORTANT**.

Remark 2.1. Intriguingly and intuitively,

$$\langle H \rangle = E.$$

Also, if the equation yields an infinite collection of solutions $(\psi_1(x), \psi_2(x), \cdots)$, each with its associated value of the separation constant $(E1, E2, \cdots)$; thus the wave function is:

$$\Psi(x,t) = \sum_{n=1}^{+\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}.$$

Particularly,

$$E_n \geq 0 \text{ for all } n$$

2.2 The infinite square well

Suppose

$$V(x) = \begin{cases} 0 & \text{if } 0 \leq x \leq a \\ \infty & \text{otherwise} \end{cases}.$$

Theorem 2.2. Inside the well, we have

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

and

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right).$$

Property 2.1. $\psi_n(x)$ has some interesting and important porperties:

1. They are alternately even and odd, with the respect to the center of the well.
2. They are mutually orthogonal (i.e., $\displaystyle\int \psi_m(x)^* \psi_n(x)\, \mathrm{d}x = \delta_{mn}$) where δ_{mn} is **Kronecker delta**:
$$\delta_{mn} = \begin{cases} 0, & \text{if } m \neq n \\ 1, & \text{if } m = n \end{cases}.$$
3. They are complete by Dirichlet's theorem.

2.3 The harmonic oscillator

Let

$$V(x) = \frac{1}{2}m\omega^2 x^2.$$

Here I will introduce 2 entirely different approaches to this problem. The first is a diabolically clever algebraic technique and the second is a straitforward "brute force" solution.

2.3.1 Algebraic method

To begin with, let's rewrite the EQ. in a more suggestive form:

$$\frac{1}{2m}\left[\left(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\right)^2+(m\omega x)^2\right]\psi=E\psi.$$

The idea is to factor the term in square brackets:

$$u^2+v^2=(u-iv)(u+iv).$$

Definition 2.2 (Ladder operator).

$$\hat{a}_\pm=\frac{1}{\sqrt{2\hbar m\omega}}(\mp i\hat{p}+m\omega x).$$

Definition 2.3 (Commutator). The commutator of operators $\hat{A}$ and $\hat{B}$ is

$$\left[\hat{A},\hat{B}\right]\xlongequal{def}\hat{A}\hat{B}-\hat{B}\hat{A}.$$

Property 2.2.

$$[\hat{a}_-,\hat{a}_+]=1.$$

Theorem 2.3. If ψ satisfies the Schrodinger's EQ. with energy E, then $\hat{a}_+\psi$ satisfies the Schrodinger's EQ. with energy $E+\hbar\omega$:

$$\hat{H}\psi=E\psi\Longrightarrow\hat{H}(\hat{a}_+\psi)=(E+\hbar\omega)(\hat{a}_+\psi).$$

Similarly,

$$\hat{H}\psi=E\psi\Longrightarrow\hat{H}(\hat{a}_-\psi)=(E-\hbar\omega)(\hat{a}_-\psi).$$

Proof.

$$\hat{H}=a_+a_-+\frac{1}{2}\hbar\omega.$$

□

Here, then, is a wonderful machine for generating new solutions——if we could just find one solution. Thus, we call $\hat{a}_+$ raising operator and $\hat{a}_-$ lowering operator.
But what if I apply the lowering operator **repeatly**? We will reach a state with energy less than zero. By 2.1, there is **NO** guarantee that it will be normalized.

Proposition 2.1. Thus, there occurs a "lowest rung" ψ_0 such that

$$\hat{a}_-\psi_0=0.$$

Theorem 2.4.

$$\psi_0(x) = A_0 e^{-m\omega/2\hbar\, x^2}$$

and

$$E_0 = \frac{1}{2}\hbar\omega.$$

Thus we could get

$$\psi_n(x) = A_n (a_+)^n e^{-m\omega/2\hbar\, x^2}, \text{ with } E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

where A_n are used for normalization.

Theorem 2.5. ψ_n and ψ_{n+1} should satisfy:

$$\begin{cases} a_+\psi_n = i\sqrt{(n+1)\hbar\omega} \\ a_-\psi_n = -i\sqrt{n\hbar\omega}\psi_{n-1} \end{cases}.$$

Proof.

$$\int_{-\infty}^{\infty} |a_+\psi_n|^2 \, \mathrm{d}x = (n+1)\hbar\omega$$

and

$$\int_{-\infty}^{\infty} |a_-\psi_n|^2 \, \mathrm{d}x = n\hbar\omega.$$

□

Ultimately,

$$A_n = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{(-i)^n}{\sqrt{n!(\hbar\omega)^n}}.$$

2.3.2 Analytic method

Things look a little cleaner if we introduce the dimensionless variables

$$\xi = \sqrt{\frac{m\omega}{\hbar}} x \text{ and } K = \frac{2E}{\hbar\omega}.$$

In terms of ξ and K, the Schrodinger equation reads

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}\xi^2} = (\xi^2 - K)\psi.$$

To begin with, consider that at very large ξ, ξ^2 completely dominates over the constant K, so in this regime $\mathrm{d}^2\psi / \mathrm{d}\xi^2 = \xi^2\psi$, which means that $\psi \Longrightarrow Ae^{\xi^2/2} + Be^{-\xi^2/2}$. Thus we let $\psi = h(\xi)e^{-\xi^2/2}$. Pluging ψ into Schordinger EQ., we have

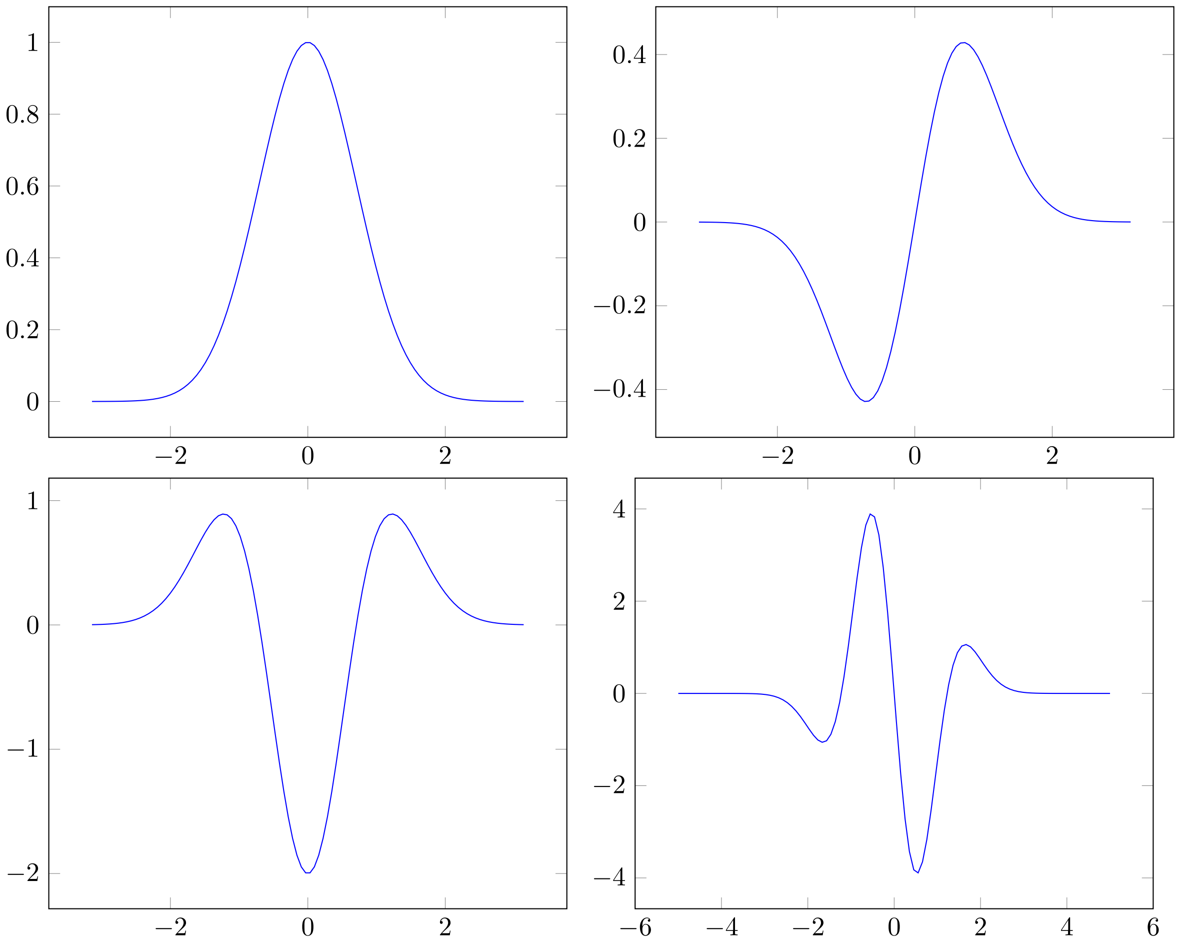
$$h(\xi) = \sum_{n=0}^{\infty} a_n \xi^n \text{ and } a_{n+2} = \frac{2n+1-K}{(n+1)(n+2)}.$$

For physically acceptable solutions (normalizable solutions), then, we must have $K = 2n + 1$.

Finally,

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}$$

where H_n is the **Hermite polynomials**.
The first four stationary states of the harmonic oscillator are as follows.



2.4 The free particle